20.1–1 IRREDUCIBLE TENSORIAL METHOD FOR MAGNETIC CRYSTALS. FULL SET OF TABLES. By M.N. Angelova, M.I.Aroyo and J.N.Kotzev. Faculty of Physics, University of Sofia, Sofia-1126, Bulgaria

The method of irreducible tensorial sets (ITS) is generalized for systems with magnetic symmetry, based on the Wigner corepresentations (coreps) and the Shubnikov antiunitary point gpoups. The following basic results are obtained: (i) generalized Racah lemma by which the ITS of an antiunitary group can be built up from the ITS of its supergroup; (ii) new form of Wigner-Eckart theorem for coreps, by which the matrix elements of quantum mechanical operators in magnetic systems can be factorized, is given; (iii) the theory of building elements of ITS for coreps is developed and their properties are investigated. An effective method for calculation of ITS coefficients is developed on the base of generalized Racah lemma. The following coefficients for all single- and double-valued coreps of all 90 Shubnikov antiunitary magnetic point groups are tabulated: (i) Clebsch-Gordan coefficients (J.Phys.A(1981) 14,1543; (1982) 15,711; (1982) 15,725); (ii) symmetrized Clebsch-Gordan coefficients the so called 3D-symbols and 2D-symbols (J.Mol. Structures(1984), in press); (iii) isoscalar factors for all possible transitions between 90 magnetic point groups, where the coreps D^j of $O(3)\times\Theta$ whith $j=0,1/2,1,\ldots,3$ are used as starting coreps (Comm.Roy.Soc. Edinburgh (1983)19, 253); (iv) 6D-symbols.
The tables are available by request from the authors.

20.1–2 SYMMETRY CLASSIFICATION OF POLYCRYSTALLINE AGGREGATES. By H.J. Bunge, Dep. of Physical Metallurgy, Univ. of Clausthal, FRG; and C. Esling, Dep. of Structural Metallurgy, Univ. of Metz, France

The symmetry description of single crystals by point groups must be generalized in order to take all possible point symmetries in polycrystalline aggregates into account.

A symmetry operation of an aggregate can be defined by a unitary transformation a^S transforming a unit vector $\vec{y}$, representative for a sample direction, into $\vec{y}^t$

$$\vec{y}^t = a^S \cdot \vec{y}, \quad |a^S_{ik}| = \pm 1, \quad \vec{y} = \{y_1, y_2, y_3\} \qquad (1)$$

and the additional requirement that $\vec{y}$ and $\vec{y}^t$ be equivalent. Equivalence of two sample directions $\vec{y}$ and $\vec{y}^t$ in a polycrystalline aggregate is defined in a statistical sense by the distribution function $I_y(h)$ of crystal directions $\vec{h}$ which are parallel to the sample direction $\vec{y}$. This function is invariant with respect to all symmetry rotations of the crystal symmetry

$$\exists_y(a^c \cdot h) = \exists_y(h), \quad |a^c_{ik}| = +1 \qquad (2)$$

If the crystals belong to an enantiomorphic class, then two such functions $I^R_{\vec{y}}(h)$ and $I^L_{\vec{y}}(h)$ are to be distinguished corresponding to right- and left-handed crystals respectively. Equivalence of two sample directions $\vec{y}$ and $\vec{y}^t$ in an aggregate can then be obtained in two different modes:

$$\left.\begin{array}{ll} \exists^R_{yt}(h) = \exists^R_y(h),\ \exists^L_{yt}(h) = \exists^L_y(h) & 1 \text{ mode} \\ \exists^R_{yt}(h) = \exists^L_y(h),\ \exists^L_{yt}(h) = \exists^R_y(h) & 2 \text{ mode} \end{array}\right\} \text{ of equivalence} \qquad (3a)$$

This contrasts with the situation in single crystals where there is only one mode of equivalence of crystal directions.

If the crystals are non-enantiomorphic, two modes of equivalence can nevertheless be defined in this case, too, by the definitions

$$\left.\begin{array}{ll} \exists_{yt}(h) = \exists_y(h) & 1 \text{ mode} \\ \exists_{yt}(a^c \cdot h) = \exists_y(h) & 2 \text{ mode} \end{array}\right\} \text{ of equivalence} \qquad (3b)$$

where a^c is one of the symmetry operations of second kind, $|a^c_{ik}| = -1$, of the crystal symmetry.

The mode of equivalence is to be kept apart from the kind of the geometrical symmetry operation defined by the sign of $|a^S_{ik}|$ in eq. (1). The second mode of equivalence has the properties of a cyclic group of second order. The symmetry of a polycrystalline aggregate, defined by eq. (1) and (3) can thus be described by a black-white point group.

References:

H.J. Bunge, C. Esling and J. Muller: J. Appl. Cryst. (1980) 13, 544-554

H.J. Bunge, C. Esling and J. Muller: Acta Cryst. (1981) A 37, 889-899

20.1–3 TO COMPLETING THE SCHEME OF THE 5-DIMENSIONAL CRYSTALLOGRAPHIC GROUPS OF SYMMETRY. By A.F.Palistrant, Dept. of Mathematics and Cybernatics, Kishnev State University, Kishnev, USSR.

The use of the methods [1,2] for employing the classical crystallographic groups of symmetry and their generalizations with the simple and 1-fold Shubnikov-Zamorzaev antisymmetry, p - and (p') - Belov-Pawley symmetry, and 32 crystallographic P-symmetries in geometrical classification (when the permutation group of the quality P is isomorphic to one in 32 crystallographic classes) to the count and modelling of the 4-dimensional groups of symmetry makes it possible to progress the principle solution of the n-dimensional geometric crystallography problem where n=5.

Indeed, the detailed calculations of the three-dimensional groups of symmetry and two-fold antisymmetry allow the numbers of the category $G_{543\ldots t}$, groups to be found. There are 17410 G_{543}; 2597G_{5431}; 4920G_{5432}; 1379G_{54321}; 624 G_{5430}; 671G_{54320}; 374G_{543210} (in accordance with the full numbers of the groups of symmetry and two-fold antisymmetry G^2_3 and G^2_{31} (ignoring enantiomorphism); G^2_{32}; G^2_{321}; G^2_{30}; G^2_{320}; G^2_{3210}).